MONDAY EVENING
Section A
Pennsylvania Convention Center
Halls D/E
Sci-Mix
E. Rosenberg, Organizer
8:00 - 10:00
5, 13. See previous listings.
25, 29-30, 48. See subsequent listings.

TUESDAY MORNING
Section A
Philadelphia Downtown Courtyard by Marriott
Grand Balloon Salon III/IV
Division of Industrial & Engineering Chemistry Graduate Student Award
M. A. Matthews, P. E. Savage, G. G. Stanley, Organizers, Presiding
8:30 ISEC 25. Amidoamine-functionalized microcrystalline cellulose-mesoporous silica composites for carbon dioxide sorption at elevated temperatures. C. Gunathilake, R. Dassanayake, N. Abidi, M. Jaroniec
8:50 ISEC 26. Factors influencing the mode(s) of facilitated ion transfer into room-temperature ionic liquids containing crown ethers. J. Wankowski, M. J. Kaul, M. L. Dietz
9:10 ISEC 27. Fundamental water and sodium chloride transport properties in a series of sulfonated crosslinked hydrogel membranes. N. Yao, D. R. Paul, B. D. Freeman
9:30 ISEC 28. Ion sorption and transport in ion exchange membranes: Importance of counter-ion condensation. J. Kameov, B. D. Freeman, D. R. Paul
9:50 ISEC 29. Synthesis of electrode materials from CO₂ and their applications in energy conversion and storage. W. Wei, Y. H. Hu
10:10 ISEC 30. 3D nanoscale imaging and photocatalytic disinfection mechanism of gram-negative and gram-positive with modified C-doped and C-P-doped TiO₂ composites under visible light radiation. J. Zheng, Y. Lin, C. Deng, Y. Huang
10:30 Intermission.
10:50 ISEC 31. Excellent capacitive deionization of large-surface area and high-conductivity carbon materials. L. Chang, Y. H. Hu
11:10 ISEC 32. Withdrawn.
11:30 ISEC 33. Product formation and kinetics of the non-isothermal methanol reforming of fumaric compounds. M. Koikh, R. F. Lobo
12:10 ISEC 35. Epoxydized soybean oil modified with renewable fatty acids as tougheners for thermosetting epoxy resins. F. Hu, G. R. Palmese
Ask Dr. Safety: Chemical Security in Research Institutions
Sponsored by CHAS, Cosponsored by CCIS and ISEC

TUESDAY AFTERNOON
Section A
Philadelphia Downtown Courtyard by Marriott
Grand Balloon Salon III/IV
Green Chemistry Innovations & Opportunities in Industry for Young Professionals
Cosponsored by CATI, CIE, CHAS, ENFL, ENVR, ORGN, POLY, PHCP, and YCC
Financially supported by Northeast Section Younger Chemists Committee (NSYCC); NSFSE; GC3
R. E. Bogg, M. Kirepos, W. A. Laval, Organizers, Presiding
1:30 Introductory Remarks.
1:35 ISEC 36. Internal structure of a chemical company. W. F. Carroll
2:05 ISEC 37. Sustainable and green chemistry opportunities in industry. D. J. Constable
2:35 ISEC 38. Green chemistry in pharmaceutical R&D in 2016. L. E. Bhatter
3:05 ISEC 39. Sustainability in chemicals manufacturing research & innovation. A. Sehgal
3:35 Intermission.
3:45 ISEC 40. Sustainability and Eastman. B. Satterfield
4:15 ISEC 41. Chemistry careers and green chemistry. G. Jimenez-Gonzalez
4:45 ISEC 42. Unintended consequences: Removing barriers to going green working in environmental compliance. F. K. Wood-Black
5:15 Concluding Remarks.

TUESDAY EVENING
Section A
Pennsylvania Convention Center
Hall D
General Posters
E. Rosenberg, Organizer
6:00 - 8:00
ISEC 43. Chemical treatment of galvanized steel by NIR photothermal conversion material. J. Baek
ISEC 44. Withdrawn.
ISEC 45. Treatment of endocrine disrupting compounds in an advanced ozone membrane reactor. Y. L. L. Luk, K. Yeung
ISEC 46. Performance of a multifunctional gel for H₂O₂ abatement in a wastewater drainage system. L. Luk, W. Han, K. Yeung
ISEC 47. Withdrawn.
ISEC 48. Study and removal of ppp level lead (II) from after wash glass bottles in beverage industry. A. Altai, A. Badshah, M. Ayub
ISEC 49. Characterisation of polymer shear thinning using fluorescence lifetime microscopy. J. Dench, N. Morgan, J. Wang
ISEC 50. Enzyme enabled one pack peroxide mediated cure for water-borne coatings. S. Anumugam

INOR Division of Inorganic Chemistry
N. Radu and S. Koch, Program Chairs
OTHER SYMPOSIUM OF INTEREST:
Small Molecules Activated by Homogeneous Metal Catalysts (see CATI, Sun)
New Trends in Organometallic Chemistry Leading to Organic Synthesis (see ORGN, Mon)
Organometallics Distinguished Author Award (see ORGN, Mon)
Industrial Innovations in Polymer Chemistry: The Interface between Inorganic Chemistry & Polymer Science (see POLY, Mon)
Advances in Teaching Inorganic Chemistry Lecture & Laboratory (see CHED, Wed)

SUNDAY MORNING
Section A
Pennsylvania Convention Center
Room 115B
Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs
S. A. Koch, Organizer
E. T. Papish, L. A. Yatsunyk, Presiding
8:30 INOR 30. Tuning insulin-sensitizing activity of polyoxovanadates derives by kinetically control their self-assemblies. K. Chen, T. Liu, Y. Wei
8:50 INOR 31. Clavanin A, a tunican anti-microbial peptide: influence of Zn²⁺ on its bactericidal activity. A.M. Angeles Boza
9:30 INOR 33. Rhodium-conjugate fluorescent probes for diagnostic of mismatched DNA. A. Nano, J.K. Barton
9:50 INOR 34. Photocatalytic properties of fluorides dyes via ruthenium(II) poly(pyridyl) ligand exchange. T.N. Rohraubag, J.K. White, C. Turro
10:10 INOR 35. Withdrawn.
10:30 Intermission.
11:00 INOR 37. Ruthenium complexes are pH-activated metallic prodrugs (pHAMPs) due to photodissociation under acidic conditions. E.T. Papish, F. Qu, J.L. Gray, J. Lundeen, Y. Kim, E.J. Merino, J.J. Paul
11:20 INOR 38. Metal coordination to ligand-modified nucleic acid triplexes. D.R. Jayarathna, H. Stout, C. Achim
12:00 INOR 40. Sodium binding DNA motif derived from a DNAzyme. J. Liu
12:20 INOR 41. Iron(I) 2-amino-6-picolyl-appended CYCLOM complex as pH-responsive paraEST MRI contrast agent. P.B. Tsvitovich, J.R. Morow

Section B
Pennsylvania Convention Center
Room 115C
Bioinorganic Chemistry: Proteins & Enzymes & Model Systems
S. A. Koch, Organizer
Y. Zhang, Presiding
8:30 INOR 42. Hydride attack on a coordinated ferric nitrosyl: A DFT investigation of the formation of a heme model-HNO derivative. R. Khadi, Y. Zhang
9:30 INOR 45. Computational study of the structure-function relationships of the fat mass and obesity associated protein. T. Karabancheva-Christova, W. Singh, J. Jinsley, C. Christov
9:50 INOR 46. Conformational dynamics and oxygen binding in non-heme iron and 2-oxoglutarate histone demethylases. C. Christov, T. Karabancheva-Christova, W. Singh
10:10 INOR 47. Hemop copper oxidase design using genetic code expansion. L. Xiaohong
10:30 INOR 48. Magnetostuctural correlation for higher-nuclearity iron(III)/oxo complexes, and application to Fe³⁺, Fe²⁺, and Fe¹⁺ clusters. K. Mitchell, K. Abboud, G. Christou

Section C
Pennsylvania Convention Center
Room 116
Organometallic Chemistry: Catalysis
N. S. Radu, Organizer
C. L. I. Tonks, Presiding

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Technical program information known at press time. The official technical program for the 252nd ACS National Meeting is available at: www.acs.org/Philadelphia2016

**SUNDAY AFTERNOON**

**Section C**

**Section D**

**Section E**

**Section F**

**Section G**

**Technical Program**
INOR 121. Light-triggered CO delivery to neoplastic target by a water-soluble and biocompatible manganese photocORM. J. Jimenez, I. Chakraborty, S. Garrington, P.K. Mascharak

INOR 122. Synthesis, characterization and in vitro anticancer studies of Ru(III), Zn(II), Cu(I) and VO(IV) complexes. P.A. Aljadeff

INOR 123. Polypryridyl Ru(II) complexes containing dimine-quinoxine ligands for dual reactivity. L.M. Lauth, T.A. White, G. Turro

INOR 124. Ternary complexes with low-denticity fluorescent Mg(II) sensors: Applications in Mg2+ and MgTAP detection. B. Pinto-Pacheco, S. Schwartz, J. Pitteloud, B. Bucella

INOR 125. Photo-activated dirhodium(II,II) complex with potential dual-binding to DNA. R. Ahlenius, G. Turro

INOR 126. Computational study of intermolecular interactions between L-cysteine and 2-mercaptopyrimidine using DFT, QTAIM, and NBO methods. I. Morkan, A. Morkan, H.C. Yazici, E. Gül, S. Tanyıldız, N. Öztürk

INOR 127. Prevention of toxic heavy metal poisoning by chelation. C.P. Kalatikite

Section E
Pennsylvania Convention Center
Room 118B

Organometallic Chemistry: Applications to Organic Transformations
N. S. Radu, Organizer
M. L. Neidig, N. C. Tomson, Presider
1:30 INOR 92. Readily prepared, scalable, and air-stable cobalt pre-catalysts for C-H borylation. N. Leonard, P.J. Chirik
2:10 INOR 94. Studies toward mild palladium(II) catalyzed arylation fluoromethylation. D. Ferguson, J.R. Bour, M.S. Sanford
2:30 INOR 95. Transmetallation and reductive elimination from isolable organometallic Ni3 complexes. E.A. Meucci, N. Camasso, M.S. Sanford
2:50 INOR 96. Direct generation of oxygen-stabilized radicals by H transfer from transition metal hydrides. J. Kuo, J. Hartung, A. Han, J.R. Norton
3:10 INOR 97. Highly chemoselective cobalt catalyst for the hydroisolation and hydroboration of alkenes. A.O. Ibrahim, S.W. Entsminger, A. Fou
3:30 INOR 98. Cobalt-catalyzed arene C(sp2)-H borylation: Scope, mechanism, and distinctions from previous metal catalysts. J. K. Obligacion, S.P. Semproni, I. Pappas, P.J. Chirik
4:10 INOR 100. Base-metal-catalyzed polyborylation of C(sp2)-H bonds. W.N. Palmer, P.J. Chirik

Section F
Pennsylvania Convention Center
Room 118B

Main Group Chemistry
T. W. Hudnall, Organizer
C. M. Thomas, Presiding
1:30 INOR 101. Coordination of N-heterocyclic phosphorus (NHP) cations to cobalt using a bidentate NHP/phosphate ligand. M. Bzopalco, C.M. Thomas
1:50 INOR 102. Chelating ligands incorporating reactive N-heterocyclic phosphorus cations. C.M. Thomas, M. Bzopalco, D.A. Evers, A. Poltas
2:10 INOR 103. NaOCP as a synthon in low-coordinate phosphorus chemistry. R.J. Gillard, R. Suter, Z. Benkő, J.D. Protasiewicz, H. Grötzmacher
2:30 INOR 104. N-heterocyclic carbones (NHCs): A new platform for activation of small molecules. E. Lee
2:50 Intermission.
3:00 INOR 105. N-heterocyclic carbone-phosphonides: Applications in the stabilization of reactive main-group and transition metal fragments. A. Dodd
3:40 INOR 107. Facile incorporation of chirality in heteroleptic pyridyl aluminium complexes. R. Garcia, D.S. Wright
4:00 INOR 108. Computational design of novel low-valent zinc complexes with Zn–Zn bonds. X. Wang

Section G
Pennsylvania Convention Center
Room 119C

Lanthanide & Actinide Chemistry
A. De Bettencourt Dias, Organizer
H. Je, H. Liu, Presider
1:30 INOR 109. High-symmetrical 12-coordinated luminescent europium(II)-containing salt. Y. Yuan, L. He, G. Tao
2:10 INOR 111. Specific recognition of lanthanide ions by DNA. J. Liu
2:50 Intermission.
3:00 INOR 113. Luminiscient terbium complex derived from dialkyldihydride ligand: Synthesis, characterization, structure and their fluorophoric properties. R. Chau, P. Elizondo, C. Mesa, H. Lao, A.A. Kukoyi
3:40 INOR 115. Element selective extraction using polynitrogen ligands in inionic liquid. J. Dehaudt, N.J. Williams, H. Luo, S. Dai

SUNDAY EVENING

Section A
Pennsylvania Convention Center
Hall D

Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs
S. A. Koch, Organizer
5:30 - 7:30

INOR 116. Incubation of Leishmania tarentole with vanadium oxides to assess their potential as therapeutic drugs. C. Wallace, C.C. McLauclan, M.A. Jones


INOR 118. Cytoxic and DNA-binding studies of organophosphorus compounds of amino acids. M. Stevenson, S. Pramanik, S.K. Mandal

INOR 119. Eradication of human breast cancer cells through trackable light-induced CO delivery from a designed photocORM entrapped within mesoporous silica nanoparticles. I. Chakraborty, S. Garrington, J.H. Hauser, S. Oliver, P.K. Mascharak

INOR 120. Development of BODIPY-based fluorescent sensors for the detection of intracellular Mg2+. Q. Lin, B. Bucella

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INOR 134. Fast growth of sub-centimeter single crystal graphene under the fold- 3D copper foil bridge. H. Wu, Z. Lue
INOR 135. Computational and experimen- tal investigation of the release of nitric oxide from s-nitrosothiols, mediated through metal organic framework catalysis events. K. Taylor, T.M. Wheat, T. Li, A.W. Maverick, R. Kumar
INOR 136. Periodically ordered inorganic nanostructures from self-assem- bled block copolymer composites. H. Wakayama, H. Yonekura, Y. Kawal
INOR 137. Synthesis of MoO4 micro- crystals and their application in water treatment. S. Chuang, S. Li
INOR 138. Controlled synthesis and microwave electromagnetic prop- erties of hcp-Co flakes. N. Chen, J. Jiang, C. Xu, L. Zhen
INOR 139. Investigating the bonding between metal-oxide supports and metal nanoparticles. A.S. Rosas, C.A. Strayc, H. Wightman, S. Magd
INOR 141. Fabrication of conduc- tive PEDOT wrapped electro- spun PMMA fibers. S.M. Boyce, L. Young, W.E. Bemier, W.E. Jones
INOR 142. Grafiting and polymerization on Perovskite-based nanosheets. S. Alkbarian-Tefaghi, J.B. Wiley
INOR 143. Scandium-based metal-organic frameworks for carboxylation of epox- ides. B. James, A. Matzger, M.S. Sanford
INOR 144. Preparation of 2D metal-organic framework (MOF)-graphene oxide composite for gas adsorp- tion. Z. Li, W. Chen, K. Yeung
INOR 145. Compresive properties of metal-organic framework (MOF) aero- gels. Z. Liu, W. Chen, W. Han, K. Yeung
INOR 146. Electrochemical analysis of Fe-doped anatase nanoparticles for Li- and Na-ion battery applications. J. Gollap, S. Naik, B.D. Fahman
INOR 147. Assessment of the Li capacity of silicon-doped carbonaceous nano- structures. M. Shokh, B.D. Fahman

Section C
Pennsylvania Convention Center Hall D

Inorganic Catalysts
S. A. Koch, Organizer
5:30 - 7:30
INOR 149. Reactivity and mechanis- tic understanding of metal-nitride complexes toward NH, activa- tion. M. Keener, G. Manard
INOR 150. Frustrated solution struc- tures can enhance electron trans- fer rate in layered manganese oxide materials. R.K. Bhullar

INOR 152. Main group-transition metal communication for oxidative catalysis. C.J. Kirby, G. Manard
INOR 154. Photocatalytic metal-organic frameworks for 2,2,2-trifluoroethanol for 3D printing of styrenes. X. Yu, S. Cohen
INOR 157. Investigating the role of redox load distribution in oxidative catalysis. C. Hunt, G. Manard
INOR 158. Tethering metal-centered radicals for substrate activations and catalysis. S. Day, B.B. Wayland, M. Zdilla
INOR 159. Modified Tris(pyridyl)ethy- lamine (TPMA) and tnn2(dimethyl- aminoo)ethane (MeTREN) hybrid ligand for the use in copper mediated atom transfer radical addition (ATRA). A.J. Rupprecht, M. Novak, T. Pintauer
INOR 160. Development of novel and highly efficient copper catalysts for atom transfer radical addition (ATRA). M. Novak, A. Kaur, T. Pintauer
INOR 161. Hydrogenation of ketones using ammonia borane and dimethyl- aminoborane as a hydrogen donor. S. Tanyildizi, I.A. Morkan, S. Ozkar
INOR 163. CMK-3 supported NiPd alloy nanoparticles and their synerg- istic effect on catalytic activity. A. Kim, H. Park, J. Park, K. Park
INOR 164. Preparation of ordered mesoporous copper oxide nano- structures with enhanced catalytic properties. A. Kim, S. Jiang, K. Park

Section D
Pennsylvania Convention Center Hall D

Main Group Chemistry
T. W. Hudnall, Organizer
5:30 - 7:30
INOR 167. Role of catalysts in the design of new borane architectures. D.M. Schubert, D. Neiner, M.E. Bowden, M. McCray
INOR 168. Tuning the electronic param- eters of H-heterocyclic carbodi- mides with phenyl boron byg group. W. Liu, G. Chu
INOR 170. Silylene-stabilized boron cata- lysts. H. Tsai, C. Chu
INOR 171. Tuning phosphorescence via number and position of methoxy substituents in difluoroborin(3-diketo- rates. M.L. Daly, C.A. DeRosa, T.P. Butler, W.A. Morris, C. Kerr, M. Sabat, C. Fraser
INOR 172. Enhancement of electron-de- ficient character of organoboron macrocycles. N. Basar-Kizalı, F. Jaakle

Section E
Pennsylvania Convention Center Hall D

Nanomaterials in Biology & Medicine
J. Galan-Mascaros, K. Sorasaenee, Organizers
5:30 - 7:30
INOR 173. Multicolor-diffused luminous- dianionene(3-diketo-ylene glycol)-poly(lactic acid) block copolymer nanoparticles. C. Kerr, C.A. DeRosa, M.L. Daly, C. Fraser
INOR 174. Surface functionalized metal-oxo polymer nanobeads as potential T1 contrast agents with dual reporting capability. V.A. Dahaynake, B.L. Stoll

Section F
Pennsylvania Convention Center Hall D

Organometallic Chemistry: Catalysis
N. S. Radu, Organizer
5:30 - 7:30
INOR 176. Nickel complexes of depo- tated HN(CH2CH2P), and their reactivity. N.P. Nambukara Wellala, J. Luebking, J.A. Krause, H. Guan
INOR 180. Upgrading isopentane to hydrocarbons through selective hydrocarbon metathesis. T. Betley, J.W. Hite, I. McKendry, A.C. Thenuwara, S. Shumlas

Radiochemical and Radiopharmaceutical Chemistry
Sponsored by FLUO, Co-sponsored by INOR, MEDI, NUCL and POLY

MONDAY MORNING

Section A
Pennsylvania Convention Center Room 115B
Di Young Investigator Awardees: Where Are They Now?
C. C. Cummings, J. D. Prosekiewicz, T. W. Warren, Organizers, Presiding
9:00 Introductory Remarks
9:10 INOR 190. Metal-ligand multi- ple bonds, extracting function from electronic structure. T. Betley
9:35 INOR 191. Solid-state chemistry career in undergraduate and PhD research programs. R.T. Macaluso
10:00 INOR 192. Bioinspired oxidative reac- tion: From Cu to Pd and Ni. L.M. Mirica
10:50 Intermssion
11:00 INOR 194. Inexpensive architectures for the production of fuels from carbon dioxide and sunlight. J. Rosenthal
11:50 INOR 196. From elemental phos- phorus to nanoscale phosphides and many things in between. B.M. Cossart
Section B
Pennsylvania Convention Center
Room 115C
Inorganic Chemistry Lectureship
J. D. Protsasiewicz, W. B. Tolman, Organizers, Presiding
8:30 INOR 197. Application of data mining for the investigation of coordination chemistry of salts and polyelectrolytes with phosphate and the ribosome. D.C. Graus, C.C. McLaughlan
9:05 INOR 198. Learning about dinuclear reactions using synthesis, spectroscopy, and theory. P.L. Holland, S.F. McWilliams, K. Grulke
9:45 INOR 200. How is metal covalency reflected in ligand field parameters? F. Nesse, E. Suturina, M. Atanasov
10:10 Intermission.
10:20 INOR 201. Transforming workhorse electron transfer proteins into energy-converting metalloenzymes. H.S. Shafat, J.W. Slater, A. Manesis, H. Monaco, R.C. Schneider
11:10 INOR 203. X-ray spectroscopic studies of nitrogenase and hydrogenase active sites. S. DeBeer

Section C
Pennsylvania Convention Center
Room 116
Organometallic Chemistry: Applications to Materials & Polymer Science
N. S. Radu, Organizer
P. J. Walsh, Presiding
8:30 INOR 204. Synthesis of biodegradable polymers via ring-opening polymerization mediated by iron(I) complexes. A. Kau, J.A. Byers
9:30 INOR 207. Redox-controlled polymerization with an iron-based catalyst. A.B. Bienemann, K.R. Delle Chiaie, J. Guley, J.A. Byers
9:50 INOR 208. Secondary coordination sphere effects in heterobimetallic Ni/Zn ethylene polymerization catalysts. A. Smith, L. Tons
10:30 INOR 210. Diaryl Complexes of Ta and Nb supported by the [CF3OMe]2 NCN trinitronic pincer ligand and ROMP of norbornene. S. Venkatraman, I. Ghiurina, K. Abboud, A.S. Veige

Section D
Pennsylvania Convention Center
Room 117
Manipulation of Energy & Electron Transfer in Molecules & Devices
K. Hanson, J. T. Hupp, J. K. McCusker, G. J. Meyer (Chairman), G. F. Strouse, Organizers
D. L. Ashford, Presiding
8:30 INOR 211. Do bases in the second coordination sphere aid CO reduction? E. Fujita, L. Duan, G. Marbeck, M. Kowalszyk, D.J. Szalda, Y. Himeda, J.T. Muckerman
9:00 INOR 212. Molecular photoelectrocalystis for hydrogen evolution in water. A.J. Miller, M. Chambers, C.L. Pitman
10:00 Intermission.
11:00 INOR 215. Photocatalytic approach to C-C cross-coupling reactions. A.K. Vannucci, A. Paul

Section F
Pennsylvania Convention Center
Room 118B
Secondary Coordination Sphere Influences: Stability, Reactivity & Everything in Between
A. R. Fout, N. K. Styczynski, Organizers
C. Scarborough, Organizer, Presiding
N. C. Tomson, Presiding
8:30 Introductory Remarks.
8:35 INOR 221. Rational design of secondary coordination sphere interactions to tune redox potentials and activities of biosynthetic models of metalloproteins. Y. Lu, P. Hossainzadeh, S. Tian, A. Bhagi-Damodaran, Y. Yu, C. Cui
9:05 INOR 222. Understanding the thermodynamic requirements for utilizing proton-relays in oxygen reduction electrocatalysts. M. Pegis, N. Kumar, S. Raugel, J.M. Mayer
9:25 INOR 223. Dictating substrate binding and imparting distinct reactivity by secondary-sphere groups. N.K. Styczynski
9:55 Intermission.
10:05 INOR 224. Pincer-crown ether ligands that bridge the primary and secondary coordination spheres: Hemilability and cation binding in catalysts. A.J. Miller, L. Smith, S. Kerr, M. Kita, J. Grapida, L. Gregor
10:35 INOR 225. Separating primary and secondary coordination sphere effects through ligand modification in non-heme iron complexes. Z. Gordon, M.J. Drummond, A. Fout
10:55 INOR 226. Architectural complexity within the secondary coordination sphere. A. Borovik

Section G
Pennsylvania Convention Center
Room 118C
Understanding Cluster Catalysts Through Biomimetic Models
J. Galan-Mascaros, Organizer
K. Sosannaire, Organizer, Presiding
8:30 Introductory Remarks.
8:35 INOR 227. Multifunctional mesoporous silica nano-particles controlled by nanomachines for biomedical targeting, imaging and drug delivery. J.J. Zink
9:20 INOR 218. Predictable heating and positive MRI contrast from a mesoporous silica-coated iron oxide nanoparticle. C.L. Haynes
10:05 Intermission.
11:05 INOR 220. Novel organic nanoparticles for cancer multimodality imaging and therapy. Z. Chng

MONDAY AFTERNOON
Section A
Pennsylvania Convention Center
Room 115B
DIC Young Investigator Awardees: Where Are They Now?
C. C. Cummins, J. D. Protsasiewicz, T. H. Warren, Organizers, Presiding
1:30 INOR 236. From Y1 to Pi: Exploring alkyne hydrogenation featuring an electron-rich cobalt catalyst. A.R. Fout
2:45 INOR 239. CO Reduction at homogeneous and heterogeneous model surfaces. C.T. Sauton, M. Bhattacharya, T. Elkin, L. Mueller, F. Wang, K. Webb
3:10 Intermission.

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Section B
Pennsylvania Convention Center
Room 115C
Chemistry of Materials: Metal Organic Frameworks
C. G. Lugmar, Organizer
P. Li, C. R. Wade, Presiding
P. Larson, J. Cheney, A. F. Cozzolino
2:10 INOR 244. Structural insight into redox hopping electron transport metal organic frameworks. P. Cais-Salazar, S. Alvarado, J. C. Morris
2:50 Intermission.
3:05 INOR 246. Flexibility, defects, and disorder in soft porous crystals: Molecular insight from computational chemistry. F. Courdet, A. Boutin, A. Fuchs
Section C
Pennsylvania Convention Center
Room 116
Coordination Chemistry: Characterization & Applications
S. A. Koch, Organizer
M. P. Jensen, C. H. Mahler, Presiding
1:30 INOR 264. Solvent cage effects: Predicting the cage recombination efficiency using microsyringe. J. Barry
2:10 INOR 261. Tunable vanadium(IV) complexes as molecular quantum memories. J. Zadrożny, M. D. Krzyaniak, D. E. Freedman
2:30 INOR 252. Fe(II), Co(II), and Ni(II) complexes of macrocycles with imidazolate pendant for Paramagnetic MRI applications. P. J. Burns, J. R. Morrow
2:50 INOR 253. Mechanistic investigation of nitrogen group transfer for the group 6 metal imido complexes incorporating a vertical series of group 14 substituents, \(-\{\text{C}_2\text{H}_2\text{N}M\text{[N(C)(C)]\text{Me}[N(P)]}\}(\text{NEMe})_3\) = Mo – W – E = – C, Si and Ge. R. Thompson, A. Kanne, P. Zavalij, A. N. Venedikov, L. R. Sita
3:30 Intermission.
3:40 INOR 255. Structural characterization of thiochromic and spin equilibria in Ni(dted,Cl)2. M. P. Jensen, I. A. Affaraj, V. G. Young
4:00 INOR 256. Quantitative structure-activity relationship studies of cobalt pynosphosphate complexes against Mycobacterium tuberculosis. T. J. Greenfield, R. Doyle
5:00 INOR 259. Inert atmospheric in-situ photo-CORFs for aerobic palladium-catalyzed carbonylation. L. M. Bensamar, S. C. Wallen
5:20 INOR 260. Activation of dinitrogen, ammonia, hydrazine and water by a terpyridine bisphosphine molybdenum platform. M. J. Bzdak, S. Guo, P. J. Chirik
Section D
Pennsylvania Convention Center
Room 117
Manipulation of Energy & Electron Transfer in Molecules & Devices
K. Hanson, J. T. Hupp, J. K. McCusker, G. J. Meyer, K. S. Schanz, G. P. Strouse, Organizers
K. Omberg, Presiding
1:30 INOR 261. TATB texture effects: Anisotropy in a plastic bonded explosive. D. G. Thompson, R. B. Schwarz, C. Liu, L. G. Hill, G. W. Brown, R. DeLuca
2:00 INOR 262. Strain functional for characterizing atomic geometries and deformation processes. E. M. Kober
2:30 INOR 263. New paradigms for old molecules: Polypyrrolidin ruthenium complexes as antibacterial agents for drug-resistant pathogens. R. Keene
3:00 INOR 264. Research summary: The Meyer research group. T. J. Meyer
3:30 Intermission.
4:30 INOR 266. MLCT excited states of poly(pyridyl) ruthenium(II) and osmium(II) complexes in ionic nanoparticles. A. to
Section A
Pennsylvania Convention Center
Room 115B
Inorganic Nanoscience Award
S. E. Skrabalak, Organizer, Presiding

8:20 Introductory Remarks.
8:30 INOR 289. Synthetic inorganic nanoscience: A platform for covering new materials and turning cartoons into reality. R.E. Schaad
9:30 INOR 291. Precise chemical, physical, and electronic nanoscale contacts. P.S. Weiss
10:00 INOR 292. Dislocation-driven growth of nanomaterials and lead halide perovskite nanowires lasers. S. Jin
10:30 Intermission.
11:15 INOR 294. Metal–ligand chemistry in multivalent nanoparticle synthesis and performance. J. Millstone
11:45 INOR 295. Seed-mediated co-reduction as a route to Pd-Cu nanostructures. E.S. Skrabalak

Section B
Pennsylvania Convention Center
Room 115C
Chemistry of Materials: Synthesis & Properties
C. G. Luskma, Organizer
A. P. Purdy, Presiding
8:30 INOR 296. Inorganic solvent-processing thermosetting materials from reactions of PINCs, with dicyanamides. A.P. Purdy, B.L. Chaloux, J.P. Yessenov, A. Epshteyn
8:50 INOR 297. Novel group IV polyazido compounds. P. Deokar, R.M. Halges, K.O. Christe
9:10 INOR 298. EuS-ZnS Core-shell nanocrystals: Synthesis and magnetic properties. D.J. James, S.L. Stoll
9:50 Intermission.
10:05 INOR 300. Synthetic, structural and magnetic studies of new Mn3, Mn4 and Mn5 clusters from the use of methyl-2-pyridyl ketone oxime in manganese phosphonate and phosphonate chemistry. O.A. Adeyako, B. Aboud, G. Christou
10:25 INOR 301. Synthetic approaches to samarium chalcogenide nano-materials. S.E. Ingram, S.L. Stoll
10:45 INOR 302. Recent progress in cluster based materials. S.L. Stoll

Section C
Pennsylvania Convention Center
Room 116
Industrial Inorganic Chemistry
N. S. Rada, J. F. Walser, Organizers, Presiding
8:30 INOR 304. Stabilized alkali metals: All of the bang, none of the boom! S.M. Bellows, J.R. Vargas, R.A. Fischer
9:00 INOR 305. Precursors for strained silicon: Volatile higher silicon compounds. B. Arlks, Y. Pan, G.L. Larson
9:30 INOR 306. From bench to bottle. H. Nienaber
10:00 INOR 307. Probing the structure and reactivity of metalloocene catalysts. K.M. Clark, A. Hook, M. Foody, B. Liu
11:00 INOR 309. Enabling modern transition-metal catalysis in drug discovery and development using high-throughput experimentation. S. Dreher
11:30 INOR 310. Combined high-throughput and mechanistic approach to the development of catalytic reactions for the synthesis of active pharmaceutical ingredients. D. Leitch

Section D
Pennsylvania Convention Center
Room 117
Manipulation of Energy & Electron Transfer in Molecules & Devices
10:00 INOR 313. Dipoles at molecule-semiconductor interfaces: energy level alignment and charge transfer properties. E. Galoppini
10:00 Intermission.
11:30 INOR 317. Transition metal complexes as electron mediators in dye sensitized solar cells. C.A. Bigioni

Section E
Pennsylvania Convention Center
Room 116A
Nanomaterials in Biology & Medicine
J. Galan-Mascaros, K. Sorasaenee, Organizers
D. Cormode, Presiding
8:30 INOR 318. Metal organic frameworks as nitric oxide scavengers for the improved biocompatibility of medical devices. M.M. Reynolds
10:00 Intermission.
11:00 INOR 321. Nanostructured metal fuels and iodine oxides for defeating bio-agents. T.P. Welts

Section F
Pennsylvania Convention Center
Room 118B
Secondary Coordination Sphere Involvements: Stability, Reactivity & Synthesis in Between
A. R. Foot, C. Scarbrough, Organizers, N. K. Szymczak, Organizer, Presiding
J. D. Gilbertson, Presiding
8:30 INOR 322. Anion reduction facilitated by secondary coordination sphere interactions in a non-heme system. A.R. Foot
9:00 INOR 323. Secondary sphere modifications influence reactivity in ruthenium-based (de)hydrogenation catalysts. E.W. Dahl, N.K. Szymczak
9:20 INOR 324. When two are better than one: Bifunctional catalysts that move protons for organic chemistry and energy. D.B. Grotjahn
9:50 Intermission.
10:00 INOR 325. Reactivity of metal complexes supported by ligands with functionalized pendant amines. T. Agapie
10:30 INOR 326. Cati-“ON” switch: Controlling reactivity using an iodium-hydride pincer-crown ether system. M. Kita, A.J. Miller
10:50 INOR 327. Nonheme iron complexes and the role of substrate orientation in the first and second coordination spheres. D.P. Goldberg, S. Sahu, L.R. Widge, A. McQuilken

Section G
Pennsylvania Convention Center
Room 118C
Lanthanide & Actinide Chemistry
A. De Bettenourt, Organizer, A. T. Johnson, J. Rack, Presiding
8:30 INOR 328. Progress toward isolation of a cerium(V)-imido complex. L. Solola
9:10 INOR 330. Femtosecond interlaminar dynamics in highly luminescent lanthanide nanomaterials. J. Rack, A.W. King, J. Wilkerson, B.J. Holloway
9:50 Intermission.
10:00 INOR 332. Effect of temperature independent paramagnetism of uranium(VI) ions on “NCM shifts and U(II) reduction of organic esters and amides. K.C. Mullane, P. Hebock, B. Manor, P. Carroll, E.J. Schelter
10:40 INOR 334. Concerted reductive elimination of alkyls from uranium(VI) using a redox active o-dilime ligand. S.A. Johnson, S.C. Bart, P.E. Fanwick, J.J. Kiernicki

Connectivity & the Global Reach of Chemistry: Honoring the Life & Scientific Contributions of Ernest L. Eliel
Sponsored by ORGN, Cosponsored by BMGT, CHED, CIFW, HEIT, INOR, PMSE and SCCHB
Section A
Pennsylvania Convention Center
Room 115B
Chemistry of Materials: Nanomaterials
C. G. Lukmur, R. M. Richards, B. G. Trevyn, Organizers
D. Carnevale, M. Shatruk, Presiding
1:30 INOR 335. Polycationic ligand control of the synthesis and self-assembly of colloidal nanocrystals through NMN spectroscopy. M. Mobarok, J.G. Veinot
3:30 INOR 340. Novel stibonium cations inorganic compounds. A.R. McDonald
4:30 INOR 344. Flame synthesis of MoO3 nanowires. F. Allen, L. Cui, P.M. Rao

Section B
Pennsylvania Convention Center
Room 115C
Main Group Chemistry
T. W. Hudnall, Organizer
A. F. Cozzolino, Presiding
1:30 INOR 346. Anion bonding with an electroneutral bidentate Sb(III) system. J. Qu, A.F. Cozzolino

Section C
Pennsylvania Convention Center
Room 116
Manipulation of Energy & Electron Transfer in Molecules & Devices
K. Hanson, J. T. Hupp, J.K. McCusker, G.J. Meyer, K.S. Scharne, G.F. Strouse, Organizers
J. J. Paul, Presiding
2:00 INOR 365. Photo-initiated energy transfer within metal-organic framework materials. J.T. Hupp, M.C. So, O.K. Farha, A. Peterson, S. Goswami
3:00 INOR 367. Quantum dot triplet sensitizers: A new frontier in photocatalysis. C. Mongin, S. Garakyaraghi, F.N. Castellano
3:30 INOR 368. Metal nanoparticle and Energy Transfer: Radiative vs non-radiative effects on a plasmonic particle. G. F. Strouse
3:30 Intermission.
4:00 INOR 359. Proton-coupled electron transfer processes underpinning the electrocatalytic generation of hydrogen. J.L. Dempsey, N. Elghrishi, B. McCarthy, E. Routree
4:30 INOR 360. Ultrafast dynamics in molecular assemblies for solar energy conversion. J.M. Papakonstantas
5:00 INOR 361. Nanobrush photocatalysts modified by electron and hole injecting dyes for degradation of environmental toxins. W.E. Jones

Section D
Pennsylvania Convention Center
Room 117
Nanomaterials in Biology & Medicine
K. Sorousaee, Organizer
J. Galan-Mascaros, Organizer, Presiding
2:45 INOR 365. Multimodal imaging-guided antitumor photothermal therapy and drug delivery using bismuth selenide nanomaterials. Z. Li, Yu, Y. Sun
3:10 Intermission.
3:45 INOR 367. Synthesis of dipyrromethene based and their use as chemical probes for metal ion imaging in biological systems. M. El Khatib, S. Vinogradov
4:10 Panel Discussion.
5:10 Concluding Remarks.

Section E
Pennsylvania Convention Center
Room 118
Solid-State Inorganic Chemistry
C. G. Lukmur, V. Pollavets, Organizers
A. J. Norquist, B. Zoeller, Presiding
1:30 INOR 368. Defect-dopant interactions in lanthanide-doped Gd III oxide nanocrystals: Controlling the dopant oxidation state and luminescent properties. V. Ghodsi, M. Hegde, P.V. Radovanovic
2:50 INOR 372. Magnetic semiconductor solid solutions: Eu5+I-II from core- and Eu1-xSmxI-II (O) and Mn2+I-II complexes. I. O. Kha, I. P. Schuster, E.S. Wiedner
3:30 INOR 374. Complex metal nitrides grown from Co/Li flux. M. Dickman, S.E. Lattuner
4:50 INOR 378. Tunable optical properties via a solid-solution for persistent luminescent applications. E. Finley, A. Cobb, A. Duke, J. Birgich
5:10 INOR 379. Oxidative mechanochemical processing of noble metals: Solvent-free preparation of salts and coordination complexes from elemental palladium and gold. L. De, T. Frisic
Cooperative Cosponsorship

T.A. Grusenmeyer, R.H. Schmehl


Implications of hydrophobic interactions for dye-sensitized photoelectrosynthesis cells (DSPEC)

M. Eubhart, K. Wei, T.J. Meyer

Mechanisms of oxygen bond formation in photoelectrochemical water oxidation on hematite photoanode.

W. Song, Y. Zhang, A. Liu, C. Chen, J. Zhao

Mechanistic considerations in water oxidation catalysis by ruthenium bipyridine-dicarboxylate and ruthenium bipyridine-phosphonate-carboxylate complexes.

D.W. Shaffer, J.J. Conception

Photoanode assemblies based on Ru(bda) catalysts for water splitting.

W. Altim, G.K. Shank, A. Greene, B. Wang, S. Simpson

Probing structural adaptability in templated vanadium selenates.

R. Xu, A.J. Norquist

WEDNESDAY MORNING

Section A

Pennsylvania Convention Center Room 115B

Bioinorganic Chemistry: Proteins & Enzyme Models Systems

S. A. Koch, Organizer
U.exas, P. U. d. G. Dorgan

8:30 INOR 487. Geometrical and electronic properties of the manganese(IV)/iron(III) cofactor of Chlamydia trachomatis dpa: comparison with iron(III) and manganese(III) porphyrins.

S. R. Al Muhannadi, Y. Wu, T. Meier, W. G. Nissen

9:00 INOR 488. De novo designed metalloproteins as models of radical enzymes. G. Ulas, T. Lenin, Y. Wu, G. T. Gained, W. F. Dargado


9:50 INOR 491. Crystallographic characterization of thioate-rich sites designed to control heavy metal geometries in de novo metalloproteins. L. Ruckhong, J. Stuckey, V.L. Pecoraro

10:10 Intermission

10:20 INOR 492. Advances in the preparation of redox active NiFe complexes based on NiS2xFeS1−x, as synthetic analogues of [NiFe]-hydrogenase enzyme active site. P. Ghosh, R. B. Chopik, C. Hsieh, N. Bhatnesh, M. V. Darnes

10:40 INOR 493. Withdrawn

11:00 INOR 494. Probing biomolecular copper(i) coordination equilibria from the picomolar to zeptomolar range. M. Morgan, A. H. Nguyen, A.M. McCaullum, D. Bourassa, P. Bagchi, H.L. Hancock, J. Basc, C.J. Fahlin

11:20 INOR 495. Synthetically accessible tetrapyrole metalloproteins as efficient photosensitizers of singlet oxygen. A.M. Potoopy, J. Roseenthal

11:40 INOR 496. Withdrawn.

Section B

Pennsylvania Convention Center Room 115C

Coordination Chemistry: Synthesis & Characterization

S. A. Koch, Organizer

T. R. Cook, W. S. Kassel, Presiding

8:30 INOR 497. Synthesis, characterization, and reactivity of Co(N(H2P(OH)PO3)3)M-Br complexes (M = Fe, Co, Cu). G. Culcu, C.M. Thomas

8:50 INOR 498. Heterobimetallic gold(I) complexes of substituted tripyridyl-phosphines. How substituents and choice of metal ion affect the physical properties of the metal–ligand complexes.

A. K. Franton, N. S. Pro, W.S. Kassel

9:10 INOR 499. Quasi-10 chains with metal–ligand interactions.

J. Guller, A.S. Hye, I. Browning, M.P. Shores, L. Doerner

9:30 INOR 500. Coordination-driven self-assembly of phosophorescent, active donor and acceptor building blocks into emissive metalloccages and cages.

T. F. Koo, Y. Zhang, C.E. Haake


C. Juida, T. Betley

10:30 Intermission


C. Heathman, T.S. Grimes, P.R. Zaluzki

11:00 INOR 504. Synthesis of diverse azole-containing chelating agents.


12:00 INOR 507. Understanding phospho-metal interactions in high valent systems using ligand donor parameters (LDPs). K. Aldrich, B. Billow, A.L. Odom

Section C

Pennsylvania Convention Center Room 116

Electrochemistry

B. L. Lucht, Organizer
J. Rosenthal, Presiding

8:30 INOR 508. CO2 reduction using a 3D printed flow electrolysis assembly. S.M. Velardo, J. Rosenthal

8:50 INOR 509. Improving the photo-stability of cyanine-based dimanganese complexes for electrolytic reduction of carbon dioxide. H. Kuo, T.W. Shaw, A.B. Bocarsly

184-TECH
Room 118A

10:00 INOR 512. Onset of cathodic silence in an anodic oxide film on gold. R.P. Giron, G.S. Ferguson

10:20 INOR 513. Bi-molecular oxygen or energy transfer between Ru(bpy)3 and ferrocene derivatives. E.R. Young, N. Pascalu-Leone, C. Drolen, E. Conklin

10:40 INOR 514. Photoswitchable ligand with metal-coordinated species for light harvesting. A. Raput, A.F. Cozzolino

11:00 INOR 515. Novel diffusimeter for high rate liquid diffusion, novel diffusion law, brilliant mass transfer, heat transfer, and for simulating oceanographic double diffusive convection. A. Khair, N.K. Dey, M.H. Rashid, X. Wang

11:20 INOR 516. Fabrication and characterization of mesoporous films of Cu2S, nanospaces for solar cell applications. M.E. Eidey, J.T. Conley, J.B. Baxter


Section A

Pennsylvania Convention Center Room 115B

Chemistry of Materials: Materials for Energy and Catalytic Applications
C. G. Lugmayr, Organizer
A. J. Morris, Y. N. Regmi, Presiding

1:30 INOR 555. Probing the charge storage mechanism of layer-structured MnOx and NIOx, pseudocapacitance materials using in operando Raman spectroscopy. D. Chen, M.A. El-Bayed, M. Liu

1:50 INOR 556. Synthesis of 3-dimensional graphene on multi-block nanorods array for lithium ion battery. S. Cho, S. Park

2:10 INOR 557. Water splitting photo- and thermo- and other devices incorporating the Ru(bpy)3 water oxidation catalysts. M.V. Shevde, B. Sherman, T.J. Meyer


2:50 INOR 559. Activation of sodium cobaltates for water oxidation catalysis through chemical etching. H. Ji, G. Sahasrabudhe, M. Vallon, A.B. Bocarsly, R.J. Cava

3:10 INOR 560. Effect of anisotropic properties of CuInS2 (Se,S) (Se2,S) single layered complex polycrystal photosensitive catalyst on water splitting. J.J. Prick, S. Kushwaha, J.W. Krizan, M.F. Baruch, R.J. Cava, A.B. Bocarsly

3:30 Intermission

4:10 INOR 561. Hydration dependent electrocatalytic activities of bimetallic oxides of Ni, Co, and Fe. V.N. Regmi, B.M. Leonard


4:50 INOR 563. Improvement in photocatalytic activity of p-type CuInO2. J.E. Park, J.W. Krizan, R.J. Cava, A.B. Bocarsly

5:10 INOR 564. Use of ether and siloxane functionalized ionic liquids and their mixtures as advanced electrolyte for lithium-ion batteries. D. Mandal

5:30 INOR 565. Microwave synthesis of Li2MnO3 nanocrystals for Li-ion batteries. P.A. Medina, B.D. Fahman, Y. Sun

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INOR 186-TECH

TECHNICAL PROGRAM

Section B
Pennsylvania Convention Center
Room 115C

Chemistry of Materials: Synthesis & Properties
C. G. Lumsden, Organizer
J. S. Holt, X. Sun, Presiding
1:10 INOR 566. Achieving maximum dye loading within zeolite channels. J.S. Holt, T. Dabertin
2:10 INOR 568. Organometallic chemistry: approach to crystalline tungsten disulfide. N. Zhang, A. Hock
2:50 INOR 570. Assembly of supertightly knotted metal-oxo charge transfer interactions. A. Voevodin, X. Roy, L.M. Campos
3:05 Intermission.
4:05 INOR 573. One-pot ultrafast synthesis of nitrogen and phosphorus co-doped carbon dots with dual wavelength fluorescence emission and high quantum yield. X. Sun, Y. Lei

Section C
Pennsylvania Convention Center
Room 116

Coordination Chemistry: Synthesis & Characterization
S. A. Koch, Organizer
A. Mukherjee, Presiding
1:30 INOR 574. Synthesis of coordination complexes of late transition metals: experimental and theoretical understanding. A. Mukherjee
1:50 INOR 575. Stereoeconomism in ruthenium complexes of chiral, linear tetradentate aminosulfoxide ligands. T.J. Brunke, A.R. Rheingold
2:10 INOR 576. Synthesis and reactivity of saturated N-heterocyclic thione (NHT) and selone (NHSe) derivatives of ruthenium(II) complexes with N-alkylated bisimidazole ligands. X. Roy, L.M. Campos
2:30 INOR 577. Synthesis and reactivity of saturated N-heterocyclic thione (NHT) and selone (NHSe) derivatives of ruthenium(II) complexes with N-alkylated bisimidazole ligands. X. Roy, L.M. Campos
2:50 INOR 578. Synthesis and reactivity of saturated N-heterocyclic thione (NHT) and selone (NHSe) derivatives of ruthenium(II) complexes with N-alkylated bisimidazole ligands. X. Roy, L.M. Campos
3:10 INOR 579. Synthesis and characterization of photostable ruthenium(lll) arene complexes incorporating pyridine and benzothiazole functionalized azopyrazole ligands. K.Y. Ghebreyesus
3:50 INOR 581. New ligand frame works on Rhenium: Rare modes of reactivity and the development of a highly reactive metallocyclo-o xo system. T.D. Lohey, R.G. Bergman, J. Arnold
4:10 INOR 582. Synthesis of dipyrin-cobalt imidos and their reactivity in C-H amination. Y. Baek, T. Betley

Section D
Pennsylvania Convention Center
Room 117

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals
N. S. Radu, Organizer
D. A. Laviska, Presiding
1:30 INOR 584. Polynuclear copper hydrides as catalysts for electron transfer from H2 to RhN, W.R. Morris, M.M. Sung
2:30 INOR 587. Synthesis and characterization of early-late polymetallic complexes. P. Dunn, I. Tongk
2:50 INOR 588. Isolation and reactivity of 2-methylimidazole complexes supported by a mononanionic bis(carbene) pincer platform. G. Espinosa Martinez, C. Ocampo, A. Fout
3:10 INOR 589. Synthesis and characterization of photostable ruthenium(lll)-arene complexes incorporating pyridine and benzoimidazole functionalized azopyrazole ligands. K.Y. Ghebreyesus
3:50 INOR 591. New ligand frame works on Rhenium: Rare modes of reactivity and the development of a highly reactive metallocyclo-o xo system. T.D. Lohey, R.G. Bergman, J. Arnold
4:10 INOR 592. Synthesis of dipyrin-cobalt imidos and their reactivity in C-H amination. Y. Baek, T. Betley

Section F
Pennsylvania Convention Center
Room 118B

Nanoscience
R. M. Richards, B. G. Trevyn, Organizers
L.U. Arachiche, Y. Mao, M. Mastro, Presiding
1:30 INOR 606. Observation of switchable photore sponses of a monolayer WS2-nanowires, lateral heterostructure via photocurrent spectral atomic force microscopic imaging. Y. Son, M. Li, C. Cheng, K. Wei, P. Liu, D. Wang, L. Li, M. Strano
2:10 INOR 608. Colloidal calixcaplycop (CuFeS2) nanoclusters as photother mal therapeutic agents. S. Ghosh
2:30 INOR 609. Size, shape, and phase control synthesis of crystalline and amorphous tin phosphide nanoparticles. V. Tallapally, R.J. Esteses, U.I. Arachiche
2:50 INOR 610. III-nitride nanow ove deposition on three-dimen sional architectures. M. Mastro
3:10 Intermission.
3:20 INOR 611. Doped lanthanum hafnate nanoclusters as scintillating materials. Y. Mao, M. Pahlke, K. Wahid
4:40 INOR 615. Controlled manipulation of chemically powered nanomotors by electric tweezers for cargo delivery and assembling of NEMS devices. J. Guo, D. Fan

Coordination Chemistry: Synthesis & Characterization
S. A. Koch, Organizer
J. P. Donahue, L. R. Falvello, Presiding
1:30 INOR 560. Screening 6-imino-2-[1,2,3-tiazol-4-yl]pyridines for colorimetric metal ion sensing properties. J.R. Jaganathan, J.T. Fletcher
2:10 INOR 562. Polyoxovanadate alkoxide clusters as novel redox-active ligands. F. Li, W.W. Brennessel, E.M. Matson
3:10 Intermission.
3:40 INOR 566. Synthesis and reactivity of N-heterocyclic thione (NHT) and selone (NHSe) derivatives of caffeine. M. Byson, D. Rubinovich
4:20 INOR 568. Twisted half-hexagon-shaped M(2)O(4H), cluster and its capacity for hosting closed-shell metal clusters. A. Ara, M. Garcia-Montes, R. Gonzalez, L.R. Falvello, M. Tomas

INOR
INORGANIC CHEMISTRY

WEDNESDAY EVENING

Section A
Pennsylvania Convention Center
Hall D

Coordination Chemistry: Synthesis & Characterization
S. A. Koch, Organizer
5:30 - 7:30

INOR 626. Ruthenium tris-bipyridine cage complexes as host systems for alkali and alkaline earth guests. A. Smale, A. Thomas, M. Harris
INOR 627. Synthesis of ruthenium macrocycles and ruthenium pendant host systems. C. J. Mendenhall, M. Harris
INOR 628. Iron and cobalt complexes with triazole appended macrocycles for DES applications. E. M. Snyder, J. R. Morrow
INOR 629. Synthesis of amide pendant ruthenium host systems. M. McBride, M. Harris
INOR 630. Preparation and study of rhodium based cluster complexes. L. F. Szczepura
INOR 631. Second coordination sphere stabilization of anion binding to metal complexes of a tripeptide triguanidine ligand. R. C. Searce
INOR 633. Corannulene as a tunable scaffold for synthesis of new curved polyaromatic ligands. Z. Z. C. Dubacs, S. N. Spisak, Z. Wei, M. A. Petrukhina
INOR 634. Synthesis of novel manga
cene(tetrazole)tetraazolates as potential high-energy density materials (HEDMs). G. O. Sullivan, M. Zdilla
INOR 635. Metal-dependent cation exchange in labile metal-organic frameworks. X. Wang, H. Zhou
INOR 636. Mixed-ligand approach for the design of heteronuclear bismuth-tran
tion metal precursors with discrete molecular structures. C. M. Lieberman, Z. Wei, A. S. Filatov, E. Dikarev
INOR 637. New synthetic routes in the synthesis of dimethylglyoximate cobalt (III) with some NS based donor ligands. A. A. Ajibola, J. A. Okeliy
INOR 638. Eu(lll) and Tb(ll) complexes of 2-(1,3-triazol-4-yl)pyridine-con
taining tridentate chelators: SPR study of fluorescence emission. M. D. Olenburg, J. T. Fletcher
INOR 639. Comparative study with tetrasubstituted (3H)-3-nitrophenyl imide lead (III) and analogous tin (II) as mesa burn rate phenomena complexes. C. Lundell, M. Zdilla, O. O’Sullivan, M. Gau
INOR 640. Detailed thermodynamic characterization of complexes of copper with substituted phenanthroline ligands. T. T. Thong, D. A. Vander Grieveld
INOR 641. Characterization of the self-as
dmbly of the 94-piece supramolecular nanojag (SOJ, CuO(OH)2[1110]), via modeling of spectrophotometric titrations with equilibrium restricted factor analysis. M. A. Aarden, D. A. Vander Grieveld
INOR 642. Stable magnesium phos
phonatoiminato, M[O(IP)]
Synthesis, structure, and reactivity. R. L. Gilliard, R. Ruten, H. Giedzen-Macher, J. D. Pretzschewicz
INOR 643. Withdrawn.
INOR 645. Copper(I) complexes with N-heterocyclic thioc (NHT) ligand derived from caffeine. C. Kansupada, M. Shlyon, D. Rabonovich
INOR 646. Preparation and character-
ization of luminescent lanthanide complexes containing O-donor ligand. P. K. Yuan, C. Lau
INOR 647. Stereocisomerism and the S-aryl group in ruthenium(l) dichloride com-
plexes of chiral, tetradentate aminosulfoxidioxide ligands. C. Stout, T. J. Brunker
INOR 648. Synthesis and crystallo-
graphic study of zinc and mercury complexes with a three-N-donor asymmetric pyridine-amine ligand. 2,9-di-pyridyl-2-yl-2,3,6-triazabi
cyclot(2.1.1)nonane. M. Hakimi

Section B
Pennsylvania Convention Center
Hall D

Electrochemistry
B. L. Lucht, Organizer
5:30 - 7:30

INOR 649. Elastic property on Si based anode by using organic-inorganic hybrid binder for reinforcement of adhe
sion during electrochemical process. H. Choi, P. No, Y. Lee, S. Jung, J. Choi
INOR 650. Comparison of the effect of alkali metals on the redox properties of different structures for bridged monova
cent polyanionstophosphates. J. F. Kirby
INOR 651. Investigation into the binding of Ti(IV) to microbial sideropheres and the potential effects on biofilm growth. J. K. Jones, A. Valentine
INOR 652. Electrocatotic reduction of CO, by a Mn(II) biquinoline tricarbonyl complex. V. Belkina, M. E. McInknon, D.C. Grills, J. J. Rochford
INOR 653. Protonation and electrochemical reduction of nucleoid and idrium-dinitro
INOR 654. Building bridges: Wiring redox
active transition metals to main group elements. T. Garroll, G. Menard
INOR 656. Heteromeric single-source precurso for the low-temperature preparation of the Li-rich spinel oxide. H. Han, Z. Wei, A.S. Filatov, A.M. Abakumov, E. Dikarev
INOR 657. Coordination-driven self-assem-
byd metalmetalactages for host-guest capture of organic pollutants. C. Fulgn, T.R. Cook
INOR 659. Nanostructured inorganic CZTS thin film prepared by facile solution process and its applica
tion to 3D p-n junction solar cells. S. Sung, S. Park, D. Kim, J. Kang
INOR 660. Recombinant expres
ssion, mutagenesis, and spectro
scopic characterization of archaeal ammonia monoxygenase. M. Smith, J.D. Caranto, K.M. Lancaster

Section D
Pennsylvania Convention Center
Hall D

Inorganic Spectroscopy
S. A. Koch, V.C. Popescu, Organizers
5:30 - 7:30

INOR 661. Analyzing host-guest interactions of metal-organic framework MIL-100 using spectroscopic methods. L. Hanna
INOR 663. Synthesis and spectroscopic characterization of a novel Ru(II) tris(2,2’-bipyridine) templated metal organic framework derived from 2m(II) and 1,3,5-tris(carboxymethyl)-benzene. C. McKithan, R.W. Larsen
INOR 664. Computational/experimental investigation of oxidative addition and photoinduced reductive elimination in coinage metal catalysts and aggregates thereof. Toward next-generation classes of photocatalysts. B.M. Otten, M.M. Ghimire, S. Tekuri, M.A. Omary
INOR 667. Probing small molecule interactions within metalloporphyrin based metal-organic frameworks using spectroscopic methods. H.O. Lahanas

Section E
Pennsylvania Convention Center
Hall D

Organometallic Chemistry: Applications to Organic Transformations
N. S. Radu, Organizer
5:30 - 7:30

INOR 668. Silver-mediated C-H func
tionalization of benzoquinone in the presence of secondary phosphate oximes and imines: The formations of C-N and C-P bonds. P. Hong
INOR 669. C-N Reductive elimination from isolated Pd(PV) complexes. E. Abada, P. Zavalli, A. V. Yedemnikov
INOR 670. Highly efficient photo
dyes in N,II catalyst systems for photon
to-reactive C-C coupling. A. Paul, M.D. Smith, A.K. vanNuccl

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INOR/MEDI

TECHNICAL PROGRAM

Section G
Pennsylvania Convention Center
Hall D
Organometallic Chemistry: Synthesis & Characterization—Early Transition Metals
N. S. Radu, Organizer
5:30 - 7:30
INOR 683. Synthesis and investigation of macrocyclic Cr(n) acetylide complexes: Emission properties and electron delocalization. E. Judkins, S. F. Tyler. T. F. Run

Section H
Pennsylvania Convention Center
Hall D
Organometallic Chemistry: Synthesis & Characterization—Late Transition Metals
N. S. Radu, Organizer
5:30 - 7:30
INOR 687. Functionalized imidazolate-based weakly coordinating anions paired with catonic transition metal catalysts. D. Wozniak, A. Hicks, D. O’Reilly
INOR 688. Synthesis and reactivity of phosphine ligated palladium(II)(Ar(CH3)2) complexes. D. Ferguson, J. R. Bort, M. S. Sanford
INOR 689. Accessibility and isolation of organometallic N0 complexes using a diverse set of oxidants. E. A. Meucci, N. Camasso, M. S. Sanford
INOR 691. Synthesis of high-valent nickel complexes supported by electron rich tridentate ligands. C. Ocampo, G. Espinosa Martinez, A. R. Freit
INOR 692. Withdrawn.
INOR 693. Exploring cooperatively redox chemistry using iron dipyrin pacman complexes. E. J. Johnson, C. Kleinlein, T. Betley

MEDI
Division of Medicinal Chemistry
W. Young, Program Chair

OTHER SYMPOSIUM OF INTEREST: Merck Research Award Symposium (see WCC, Sun)

Effectively Harnessing the World’s Literature to Inform Rational Compound Design (see CINF, Sun)

Chemistry For the People: Reflections from Perkin Medalists (see CHED, Mon)

SOCIAL EVENTS:
Hall of Fame Reception, 5:30 PM: Tue

BUSINESS MEETINGS:
MEDI Executive Meeting (Closed), 8:30 AM: Sun
MEDI Long-Range Planning Committee Meeting (Closed), 5:30 PM: Mon

MEDI SUNDAY MORNING

Section A
Pennsylvania Convention Center
Room 114
Renaisance of Estrogen Receptor-Based Therapy
S. Peukert, X. Wang, Organizers, Presiding
8:30 MEDI 1. SERMs and SERDs as the cornerstone of endocrine therapy in ER+ breast cancer therapy. D. McDowall, K. Cocco, S. Wardell, J. Norris
9:10 MEDI 2. Benzothiophene SERMs, SERDs, MERDs, SEMs, and SHERPs in endocrine-independent ER+ breast cancer therapy. G. R. Thatcher, D.A. Tonetti, R. Xiong, H. Patel
9:45 MEDI 3. GDC-0810: An orally bioavailable selective estrogen receptor degrader for breast cancer. X. Wang
10:20 MEDI 4. Tetrahydroisoquinolines as selective estrogen receptor degraders with good oral bioavailability in preclinical species. H. Burks
10:50 MEDI 5. Fifty shades of SERD: Designing and characterizing selective estrogen receptor degraders towards clinical candidates. G. Da Savi, J.S. Scott, S.L. Degorge

Section B
Pennsylvania Convention Center
Room 113C
General Orals
W. B. Young, Organizer
J. B. Schwarz, Presiding
10:10 MEDI 11. Discovery of potent, selective, CNS-penetrant potentiators of glycine receptors. E. Dumourot
10:30 MEDI 12. Isoform selective AMPK activators. K.O. Cameron
10:50 MEDI 13. Discovery of the potent and selective pyridine M. PAN. PF-06767835: Evaluation of efficacy and cholinergic side effects. J. Davenport
2:00 MEDI 19. Discovery of ubrogepant (MK-1602): A potent, selective and orally bioavailable CGRP receptor antagonist for the acute treatment of migraine. M.E. Fraley
4:00 MEDI 23. Discovery of a first-in-class, potent, selective and orally bioavailable inhibitor of the FTO. AAA ATPase (CB-5083). H. Zhou